Atomistic-continuum coupling within a Spacetime Discontinuous Galerkin framework

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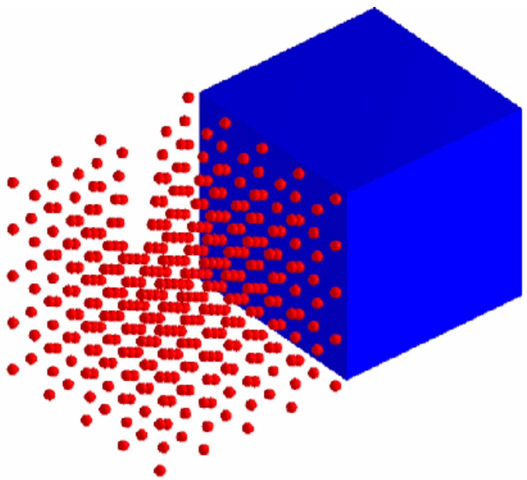
Atomistic-continuum coupling: Objective

Objective: Develop coupling formalism for solid mechanics that

1. Treats different scales
   with appropriate methods

2. Allows refinement/coarsening of scales
   in both space and time

3. Maintains compatibility and
   balance of momentum and energy



4. Eliminates unphysical reflections at atomistic-continuum interface

5. Is O(N) and parallelizable for dim≥1

6. Permits dropping in “favorite-flavor” of MD (possible restrictions on time-stepping)

7. Accomplishes all this within a consistent mathematical framework

We have partially fulfilled these objectives within the mathematical framework of an elastodynamic spacetime discontinuous Galerkin (SDG) finite element method.

Configuration space vs. phase space (discrete)

Newton's principle of determinacy and 2nd law of motion:

Initial positions and velocities of system uniquely determine entire motion of system.

$$\dot{\mathbf{p}}_i - \sum \mathbf{F}_i = \mathbf{0}\ ,\ \mathbf{p}_i = m\dot{\mathbf{u}}_i$$

Two (nearly) equivalent viewpoints:

<u>Configuration space</u>

Viewpoint:

Employ $\mathbf{u}, \dot{\mathbf{u}}$,
with $\mathbf{u}$ and $\dot{\mathbf{u}}$ interdependent

Equation of motion:

$$m\ddot{\mathbf{u}}_i - \sum_j \mathbf{F}_{ij}\left(\{\mathbf{u}_j\}\right) = \mathbf{0}$$

Viewpoint of Lagrangian mechanics

Better suited for

- General use
- Relativistic mechanics

<u>Phase space</u>

Viewpoint:

Employ $\mathbf{u}, \mathbf{p} = m\mathbf{v}$,
assuming $\mathbf{u}$ and $\mathbf{p}$ independent

Equation of motion + compatibility:

$$\dot{\mathbf{p}}_i - \sum_j \mathbf{F}_{ij}\left(\{\mathbf{u}_j, \mathbf{p}_j\}\right) = \mathbf{0}$$

$$\mathbf{p}/m - \dot{\mathbf{u}} = \mathbf{0}$$

Viewpoint of Hamiltonian mechanics

Better suited for

- Statistical mechanics
- Quantum mechanics

2-field continuum formulation: Fields

- Kinematic fields:
  - Displacement $\mathbf{u} = u_i \mathbf{e}^i,$
  - Velocity $\mathbf{v} = v_i \mathbf{e}^i, \quad \boldsymbol{v} = \mathbf{v}\, dt$
  - Symmetric strain ($E_{ij} = E_{ji}$) $\mathbf{E} = E_{ij} \mathbf{e}^i \otimes \mathbf{e}^j, \quad \boldsymbol{E} = \mathbf{E} \wedge \boldsymbol{d}\mathbf{x}$

- Dual fields
  - Momentum density $\mathrm{p} = p^i \mathrm{e}_i, \quad \boldsymbol{p} = \mathrm{p} \wedge \star \boldsymbol{d}t$
  - Stress ($\sigma^{ij} = \sigma^{ji}$) $\bar{\boldsymbol{\sigma}} = \sigma^{ij} \mathrm{e}_i \otimes \mathrm{e}_j, \quad \boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} \wedge \star \boldsymbol{d}\mathrm{x}$

- Constitutive relations

  ($\mathbf{C}$ = elasticity tensor, ρ = mass density)

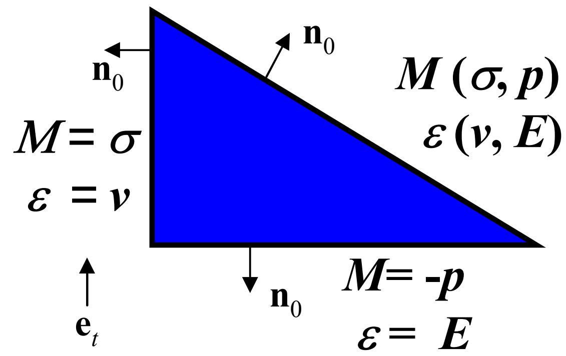
$$\boldsymbol{p} = \star \rho \boldsymbol{v}$$

$$\boldsymbol{\sigma} = \star \mathrm{C} \wedge \boldsymbol{E}$$

- Strain-velocity and stress-momentum

$$\boldsymbol{\varepsilon} := \boldsymbol{v} + \boldsymbol{E}$$

$$\boldsymbol{M} := \boldsymbol{\sigma} - \boldsymbol{p}$$



ε and $\boldsymbol{M}$ follow characteristics of wave equation

2-field continuum formulation: Energy balance

- Total energy density $\quad \boldsymbol{\Phi} = \frac{1}{2}\boldsymbol{v} \wedge \boldsymbol{p} + \frac{1}{2}\boldsymbol{E} \wedge \boldsymbol{\sigma}$

- Relationship to Hamiltonian density $\mathcal{H}$ (=spatial energy density)

$$\mathcal{H}\boldsymbol{\Omega} = \boldsymbol{\Phi}$$

- Energy flux

$$\boldsymbol{N} := -i\boldsymbol{\Phi} + \boldsymbol{iv} \wedge \boldsymbol{\sigma}$$

$\perp \mathbf{e}_t$: work done on body due to tractions

$\parallel \mathbf{e}_t$: temporal energy flow into/out of body

this is equivalent to $\quad \boldsymbol{N} = \frac{1}{2}\left(\boldsymbol{i\varepsilon} \wedge \boldsymbol{M} + \boldsymbol{\varepsilon} \wedge \boldsymbol{iM}\right)$

- Energy balance (including work done by external body forces $\boldsymbol{b}$)

$$\int_{\partial Q} \boldsymbol{N} + \int_{Q} \boldsymbol{iv} \wedge \rho \boldsymbol{b} \qquad \forall Q \subset D$$

2-field continuum formulation: Field compatibility and EOM

- Field compatibility
  - 2 fields are $\mathbf{u}$, $\mathbf{v}$ ⇒ Strongly enforce $\mathbf{E} - \mathrm{sym}\,\nabla\mathbf{u} = \mathbf{0}$
  - Split $\dot{\mathbf{u}} - \mathbf{v} = \mathbf{0}$ into strained and strain-free:
    - strain-velocity compatibility $\dot{\mathbf{E}} - \mathrm{sym}\,\nabla\mathbf{v} = \mathbf{0} \quad \Leftrightarrow \quad \mathrm{sym}\,\boldsymbol{d\varepsilon} = \mathbf{0}$
    - displacement-velocity compatibility $\dot{\mathbf{u}}_{\emptyset} - \mathbf{v}_{\emptyset} = \mathbf{0} \quad \Leftrightarrow \quad \dot{\mathbf{u}}_{\emptyset}\boldsymbol{dt} - \boldsymbol{v}_{\emptyset} = \mathbf{0}$
      (ø subscript denotes strain-free)

- Equation of motion $\nabla \cdot \boldsymbol{\sigma} - \rho\dot{\mathbf{v}} + \rho\mathbf{b} = 0 \quad \Leftrightarrow \quad \boldsymbol{dM} + \rho\boldsymbol{b} = \mathbf{0}$

- Continuum formulation from **Equation of Motion** and 2 compatibility relations: **strain-velocity** and **displacement-velocity**

Continuum formulation: Strong and weighted residual forms

- Full strong form (including jump terms):

$$(\boldsymbol{dM} + \rho \boldsymbol{b})|_Q = \mathbf{0} \qquad \text{sym } \boldsymbol{d\varepsilon}|_Q = \mathbf{0} \qquad (\dot{\mathbf{u}}_\emptyset \boldsymbol{dt} - \boldsymbol{v}_\emptyset)|_Q = \mathbf{0}$$

$$(\boldsymbol{M}^* - \boldsymbol{M})|_{\partial Q} = \mathbf{0} \qquad (\boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon})|_{\partial Q} = \mathbf{0} \qquad (\mathbf{u}_\emptyset^* - \mathbf{u}_\emptyset)|_{\partial Q} = \mathbf{0}$$

- Weight according to energy (recall flux $\boldsymbol{N} = \frac{1}{2}(\boldsymbol{i\varepsilon} \wedge \boldsymbol{M} + \boldsymbol{\varepsilon} \wedge \boldsymbol{iM})$)

- Weighted residual form (weighting functions denoted with ^):

$$\int_Q \boldsymbol{i}\hat{\boldsymbol{\varepsilon}} \cdot (\mathbf{dM} + \rho \boldsymbol{b}) \qquad + \int_{\partial Q} \boldsymbol{i}\hat{\boldsymbol{\varepsilon}} \cdot (\boldsymbol{M}^* - \boldsymbol{M})$$

$$+ \int_Q \mathbf{d}\boldsymbol{\varepsilon} \wedge \boldsymbol{i}\hat{\boldsymbol{M}} \qquad + \int_{\partial Q} (\boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon}) \wedge \boldsymbol{i}\hat{\boldsymbol{M}}$$

$$+ \int_Q k^Q \hat{\mathbf{u}}_\emptyset \, (\dot{\mathbf{u}}\boldsymbol{d}t - \boldsymbol{v}) \wedge \star \boldsymbol{d}t + \int_{\partial Q^-} k^Q \hat{\mathbf{u}}_\emptyset \, (\mathbf{u}^* - \mathbf{u}) \star \boldsymbol{d}t$$

$$= 0 \ \forall \hat{\mathbf{v}} \in \mathcal{V}_h^{Q,v} \text{ and } \hat{\mathbf{u}} \in \mathcal{V}_h^{Q,u}$$

(Function spaces are broken Sobolev spaces, $H^1(Q, \mathbb{E}^d)$)

2-field continuum formulation: Summary of properties

- Reduces to 1-field formulation with strong enforcement of $\dot{\mathbf{u}} - \mathbf{v} = \mathbf{0}$

$$\int_Q \dot{\hat{\mathbf{u}}} \cdot (\boldsymbol{d}\boldsymbol{M} + \rho \boldsymbol{b}) + \int_{\partial Q} \dot{\hat{\mathbf{u}}} \cdot (\boldsymbol{M}^* - \boldsymbol{M})$$

$$+ \int_{\partial Q} (\boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon}) \wedge \boldsymbol{i}\hat{\boldsymbol{\sigma}} \;\; + \int_{\partial Q^{ti}} k^Q \hat{\mathbf{u}}_0 \, (\mathbf{u}^* - \mathbf{u})$$

$$= \mathbf{0} \; \forall \hat{\mathbf{u}} \in \mathcal{V}_h^Q$$

- Energy converges as $h^{2p\text{-}1}$

- Momentum analytically conserved

Discrete and continuum mechanics: Physical quantities

	Atomistic	Continuum
Displacement, velocity	$\{\mathbf{u}_\alpha\}, \ \{\mathbf{v}_\alpha\}$	$\mathbf{u}, \ \mathbf{v}$
Strain		$\mathbf{E}$
Kinetic energy	$\frac{1}{2}\mathbf{v}_\alpha \cdot \mathbf{p}_\alpha$	$\frac{1}{2}\boldsymbol{v} \wedge \boldsymbol{p}$
Potential energy (density)	$V(\{\mathbf{u}_\alpha\}) = \tilde{V}\left(\{\mathbf{u}_\alpha + \mathbf{x}^0_\alpha\}\right)$	$\frac{1}{2}\boldsymbol{E} \wedge \boldsymbol{\sigma}$
Force/stress	$\mathbf{F}_\alpha = -\nabla_\alpha V(\{\mathbf{u}_\alpha\})$	$\bar{\boldsymbol{\sigma}} = \mathbf{C}\nabla\mathbf{u}$
Work	$\int dt \ \mathbf{v}_\alpha \cdot \mathbf{F}_\alpha$	$\int_{\partial Q} \boldsymbol{i}\boldsymbol{v} \wedge \boldsymbol{\sigma}$
EOM	$\mathbf{F}_{\alpha'}(\{\mathbf{u}_\alpha\}) - m_{\alpha'}\dot{\mathbf{v}}_{\alpha'} = 0$	$\nabla \cdot \boldsymbol{\sigma} - \rho\dot{\mathbf{v}} + \rho\mathbf{b} = 0$
Compatibility	$\dot{\mathbf{u}}_{\alpha'} - \mathbf{v}_{\alpha'} = 0$	$\dot{\mathbf{u}} - \mathbf{v} = 0$

SDG for discrete mechanics: Atomistic SDG (aSDG)

Investigate relationship between atomistic and continuum mechanics through development of atomistic SDG

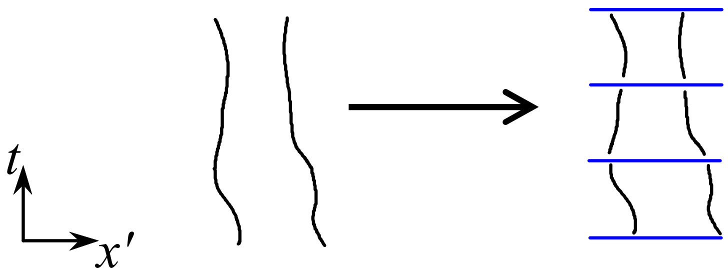
- Solution to atomistic (spatially discrete) coupled ODEs
- Finite element method in time
- “Two-field”: Treat u and v individually for each vector component of each atom

aSDG and cSDG: Equation of motion and momentum balance

- Atomic interaction is non-local force
  - Atoms interacting with one another advance simultaneously
  - Cannot use causal meshing from cSDG for implicit solution

- Divide problem into simultaneous solution on successive time intervals:

world lines of 2
displaced particles



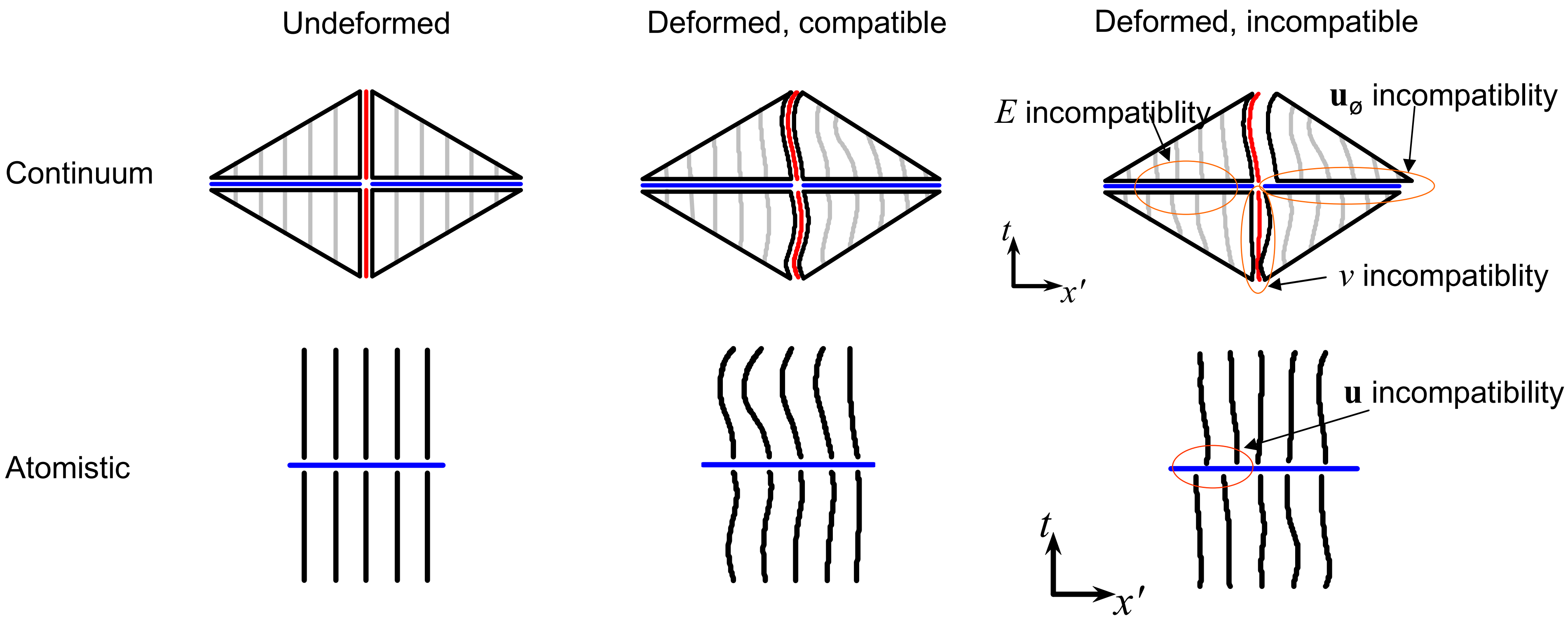
- Jump term associated with EOM is discrete momentum flow across temporal interface

- Contribution of EOM and associated jump term on $t \in (t_i , t_o)$ to aSDG

$$\sum_\alpha \left[\int_{t_1}^{t_2} dt\ \hat{\mathbf{v}}_\alpha \cdot (m_\alpha \dot{\mathbf{v}}_\alpha + \mathbf{F}_\alpha) \qquad + \hat{\mathbf{v}}_\alpha \cdot \left(m_\alpha \mathbf{v}_\alpha^{prev} - m_\alpha \mathbf{v}_\alpha \right)\Big|_{t=t_1} \right]$$

aSDG and cSDG: Kinematic compatibility

- Compatibility of atomic positions required across temporal interfaces



- Contribution of compatibility to aSDG

$$\sum_{\alpha} \left[\int_{t_1}^{t_2} dt \; k^a \hat{\mathbf{u}}_\alpha \cdot (-\dot{\mathbf{u}}_\alpha + \mathbf{v}_\alpha) \quad + k^a \hat{\mathbf{u}}_\alpha \cdot (\mathbf{u}_\alpha^{prev} - m_\alpha \mathbf{u}_\alpha)|_{t=t_1} \right]$$

Atomistic SDG: Formulation

- Full aSDG formulation:

$$\sum_\alpha \left[\int_{t_1}^{t_2} dt\ \hat{\mathbf{v}}_\alpha \cdot (m_\alpha \dot{\mathbf{v}}_\alpha + \mathbf{F}_\alpha) \qquad + \hat{\mathbf{v}}_\alpha \cdot (m_\alpha \mathbf{v}_\alpha^{prev} - m_\alpha \mathbf{v}_\alpha)|_{t=t_1} \right]$$

$$+ \sum_\alpha \left[\int_{t_1}^{t_2} dt\ k^a \hat{\mathbf{u}}_\alpha \cdot (-\dot{\mathbf{u}}_\alpha + \mathbf{v}_\alpha) \qquad + k^a \hat{\mathbf{u}}_\alpha \cdot (\mathbf{u}_\alpha^{prev} - m_\alpha \mathbf{u}_\alpha)|_{t=t_1} \right] = \mathbf{0} \forall \hat{\mathbf{u}}_\alpha, \hat{\mathbf{v}}_\alpha$$

- Properties
  - Finite element method in time for MD
  - Momentum balance analytically zero
  - Dissipates energy (like continuum) at low rate

Atomistic SDG from Continuum SDG

- All fields and mass density localized at atoms:

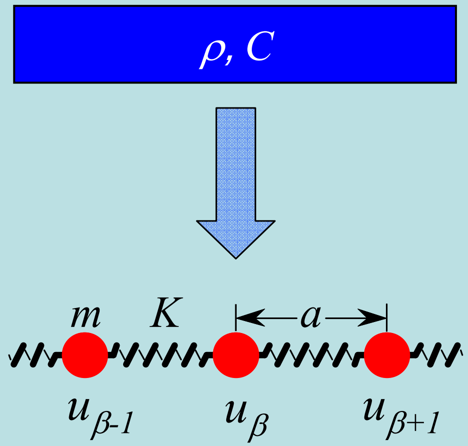
$$\rho(\mathbf{x},t) = \sum_{\alpha} \delta(\mathbf{x}-\mathbf{x}_{\alpha})\, m_{\alpha}$$

$$\mathbf{u}(\mathbf{x},t) = \sum_{\alpha} \delta(\mathbf{x}-\mathbf{x}_{\alpha})\, \mathbf{u}_{\alpha}(t)$$

$$\mathbf{v}(\mathbf{x},t) = \sum_{\alpha} \delta(\mathbf{x}-\mathbf{x}_{\alpha})\, \mathbf{v}_{\alpha}(t)$$

$$\mathbf{dp}(\mathbf{x},t) = \sum_{\alpha} \delta(\mathbf{x}-\mathbf{x}_{\alpha})\, \dot{\mathbf{p}}_{\alpha}(t)\, dt$$

Model system $(1d)$



- Stress/strain undefined—
  interactions via body forces (non-local)

$$\mathbf{d\sigma}(\mathbf{x},t) \rightarrow \rho\mathbf{b}(\mathbf{x},t) = \sum_{\alpha} \delta(\mathbf{x}-\mathbf{x}_{\alpha})\, \mathbf{F}_{\alpha}\left(\{\mathbf{x}_{\beta}(t)\}\right)\Omega$$

(recall EOM: $\mathbf{dM} + \rho\mathbf{b} = -\mathbf{dp} + \mathbf{d\sigma} + \rho\mathbf{b} = \mathbf{0}$)

Making aSDG explicit: Position update

1. Enforce continuity of displacement on time-inflow interface:

$$\mathbf{u}_\alpha^{prev}\left(t_i\right) - \mathbf{u}_\alpha\left(t_i\right) \to 0$$

2. Take explicit (independent) time-step for u, e.g. as in Velocity Verlet:

$$\mathbf{u}_\alpha\left(t_o\right) = \mathbf{u}_\alpha\left(t_i\right) + \mathbf{v}_\alpha\left(t_i\right)\Delta t + \tfrac{1}{2m}\mathbf{F}_\alpha\left(t_i\right)\Delta t^2, \quad \Delta t = t_o - t_i$$

Explicit step decouples $\mathbf{u}$ and $\mathbf{v}$

Making aSDG explicit: Velocity step

1. Take explicit time-step in $\mathbf{u}$, decoupling $\mathbf{u}$ and $\mathbf{v}$

2. Calculate force/acceleration according to $\{\mathbf{x}_\beta(t_1)\}$ and $\{\mathbf{x}_\beta(t_2)\}$

3. Lowest order: Obtain V. Verlet from velocity portion of atomistic SDG by
   - restricting $\mathbf{v}(t)$ to quadratic function space
   - integrating via Simpson's rule for 3 linearly independent $\hat{\mathbf{v}}_\alpha(t)$

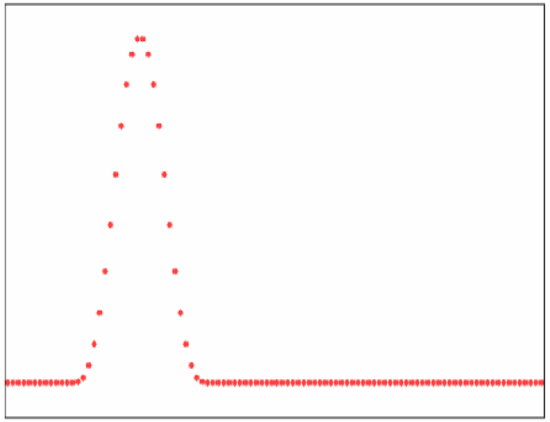
This yields

Continuity at time-inflow interface	$\mathbf{v}_\alpha^{prev}(t_i) - \mathbf{v}_\alpha(t_i) = 0$
Equation of motion at t_1, t_2	$\dot{\mathbf{v}}_\alpha(t_1) = \frac{1}{m}\mathbf{F}_\alpha(t_1), \quad \dot{\mathbf{v}}_\alpha(t_2) = \frac{1}{m}\mathbf{F}_\alpha(t_2)$
⇒ Velocity update of Velocity Verlet	$\mathbf{v}_\alpha(t_2) = \mathbf{v}_\alpha^{prev}(t_1) + \frac{1}{2m}\left(\mathbf{F}_\alpha(t_1) + \mathbf{F}_\alpha(t_2)\right)\Delta t$

Lowest order explicit approximation of aSDG coincides with Velocity Verlet

Atomistic SDG: Test case

- Implicit calculation with linear-spring interaction
- Employ different polynomial orders and compare with VVerlet
- 1d with periodic boundary conditions
- Initial condition: Pulse derived from truncated Fourier series
  - Allows comparison with analytic result, including dispersion for pure atomistc case
  - C^{∞} in continuum calculations
  - Tends not to obscure error



- Fix 100 atoms
- Vary dt as a fraction of a/c

  (interatomic spacing / maximum wave speed; dt=1.0 $a/c \Leftrightarrow$ CFL)

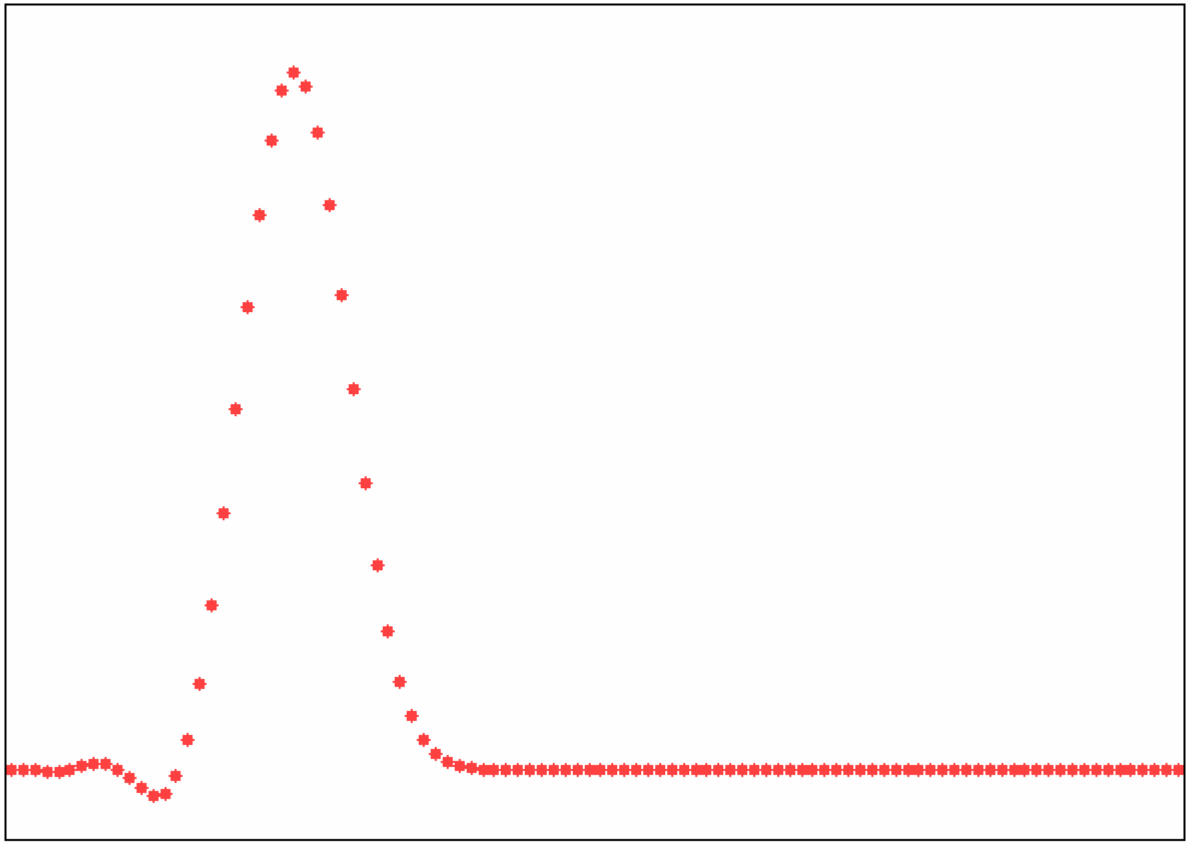
  Include timestep longer than CFL
- One set of long runs to show long-term stability

Atomistic SDG: Displacement

aSDG: 100 atoms, 3+2 dof

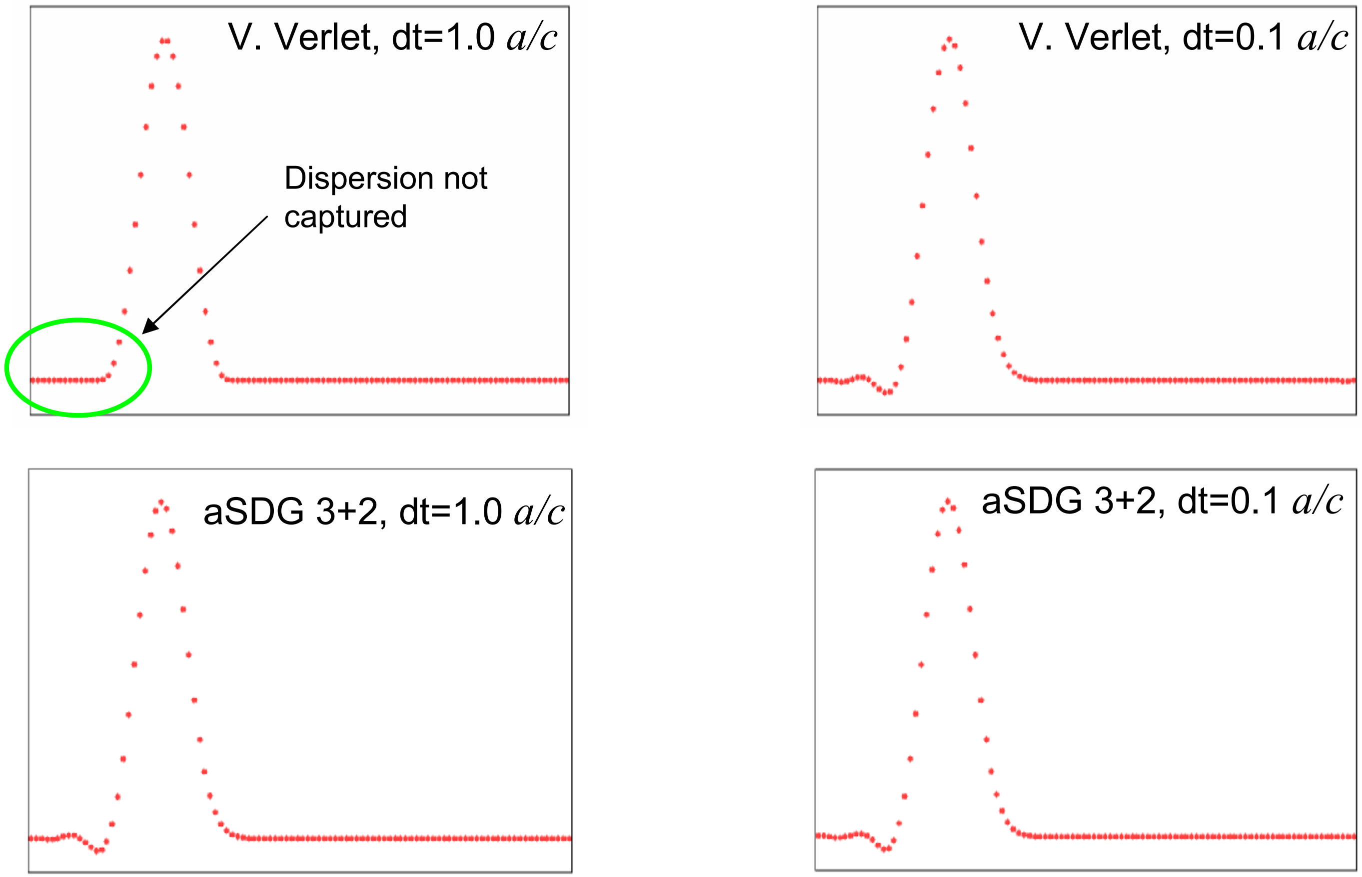
see external movie file: aSDG100at

IAsdg: Displacement t=1.0000



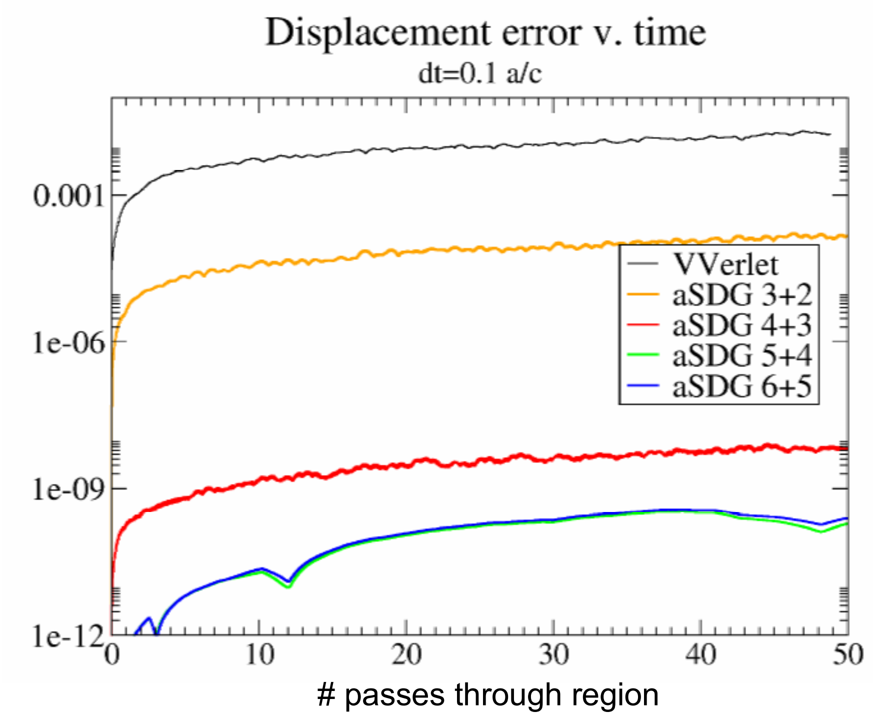
aSDG and VVerlet: Displacement error and dispersion

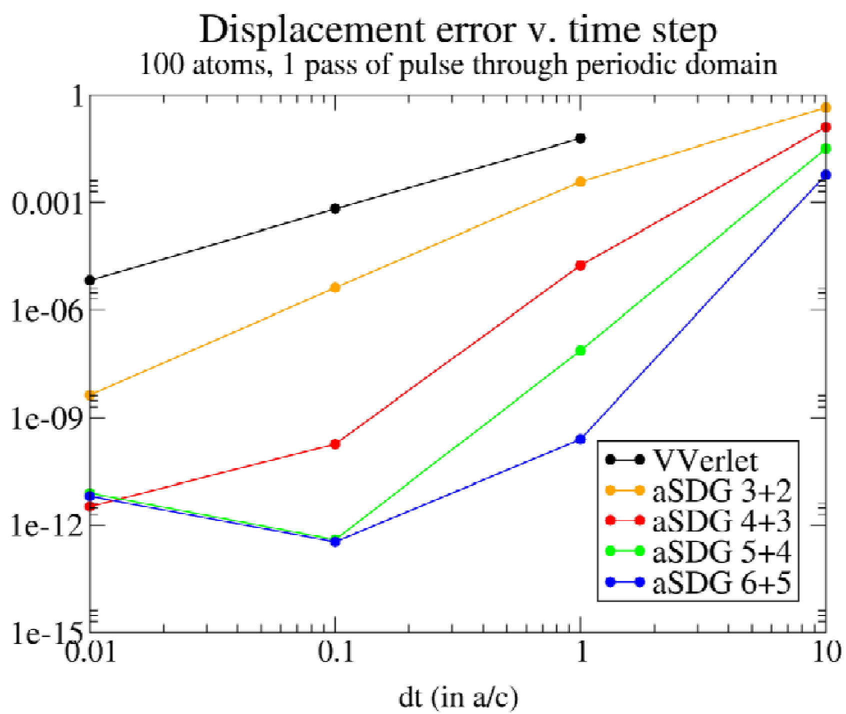
Displacement after 1 pass of pulse through periodic domain (100 atoms)



- Velocity Verlet has trouble resolving dispersion for dt=1.0 case.

aSDG: Displacement error



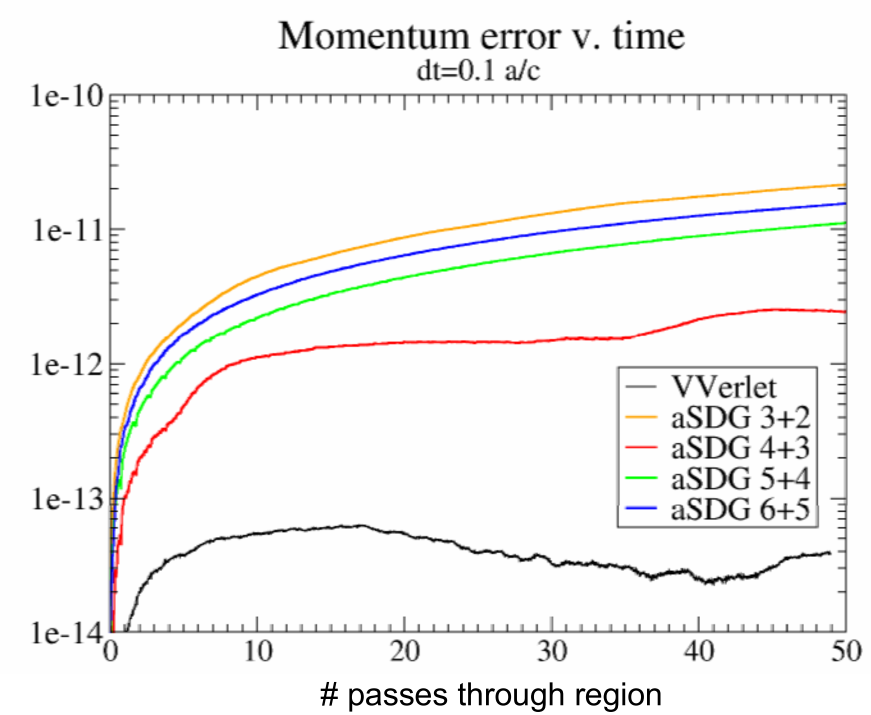


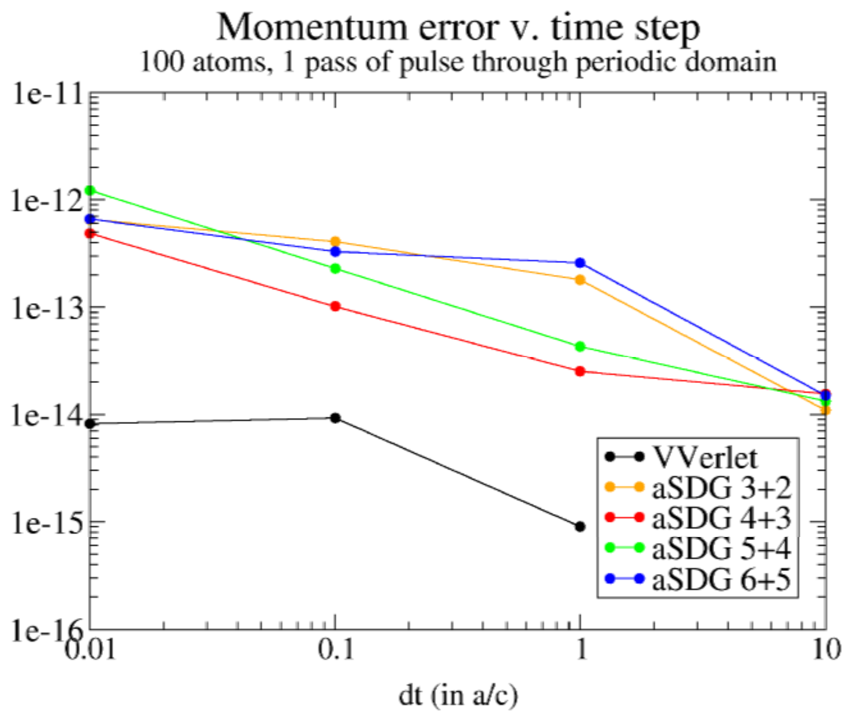
- NOTE: On all plots, '$a+b$' signifies a dof for u, b dof for v.

  E.g. for 3+2, displacement ~ t^2, velocity ~ t

- Error defined as (L_∞ error)/($u_{maxInit}$-$u_{minInit}$)

aSDG: Momentum error

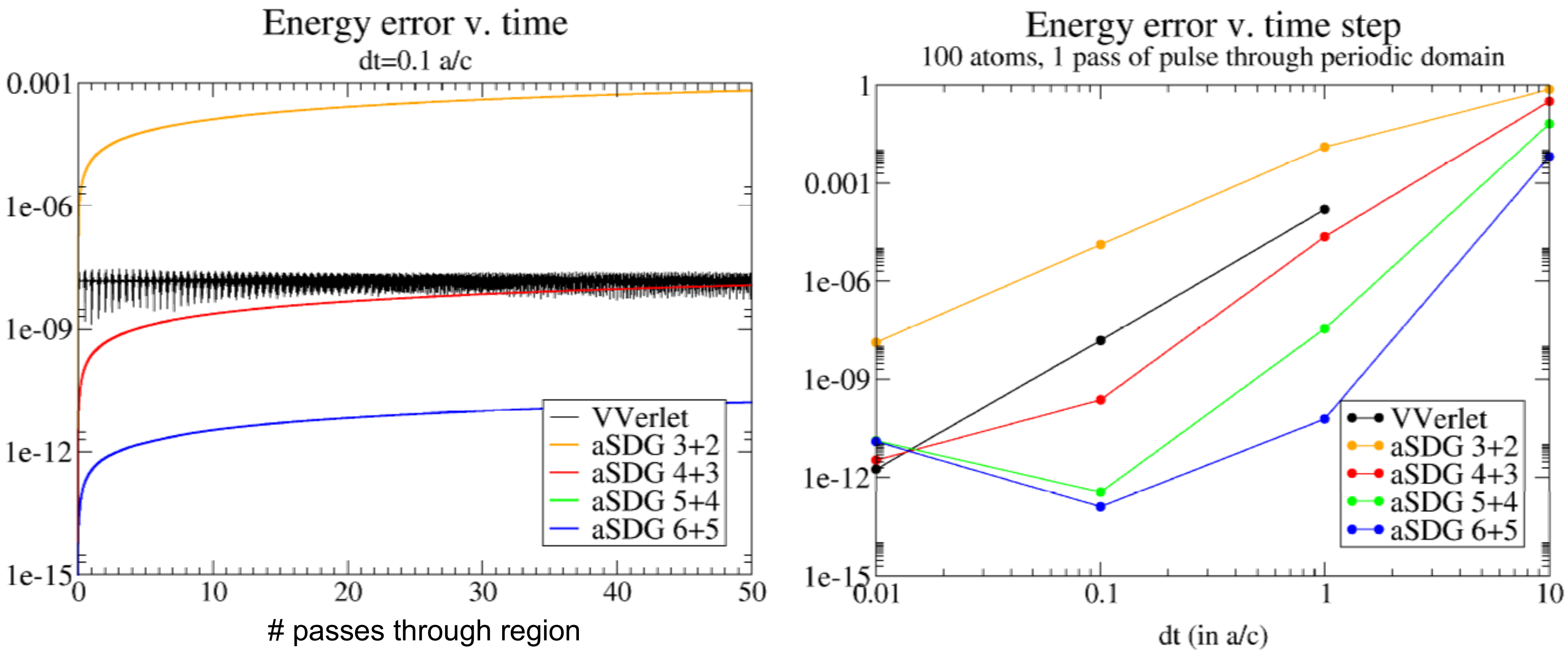




- Initial momentum is zero, so error is absolute error in total momentum, normalized by L_2-norm of initial momentum

- Analytically aSDG conserves momentum exactly, so all error due to finite precision arithmetic

aSDG: Energy error



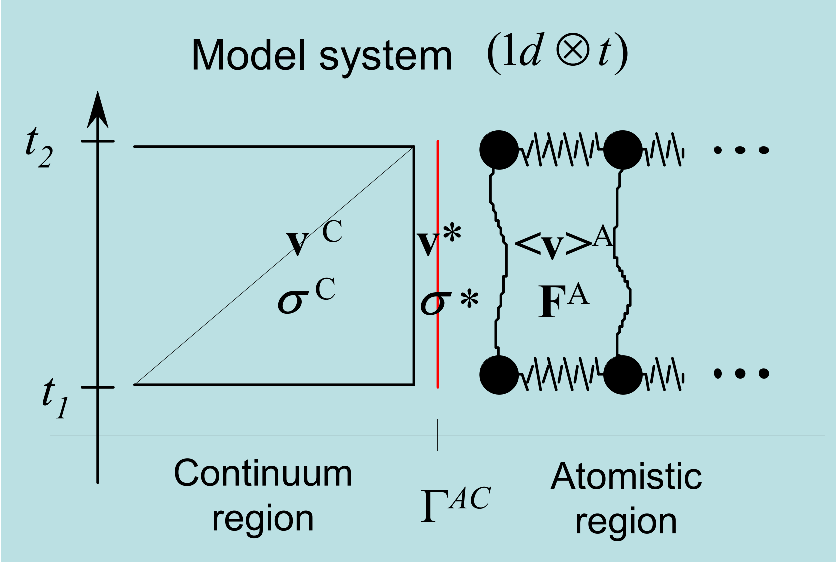
- Absolute energy change normalized by initial energy magnitude
- Non-drifting energy of V. Verlet well-known, but incompletely understood
- aSDG is energy dissipative: plots are of normalized, absolute error

Discrete mechanics and Atomistic SDG: Summary

- Primary difference between continuum and atomistic methods enters through non-local, discrete nature of interatomic interaction
  - Forces instead of stress
  - Forces act non-locally, requiring different approach to causality
  - Strain not well defined
- Atomistic SDG offers family of higher order schemes for MD
- aSDG shows similar momentum and energy properties to cSDG
- Future investigation of higher-order explicit atomistic methods planned

Coupling: Atomistic and continuum SDG

- 2-field SDG is governing mathematical model
- Employ continuum 2- or 1-field SDG in continuum region
- Couple through flux compatibility relations at Γ^{AC}

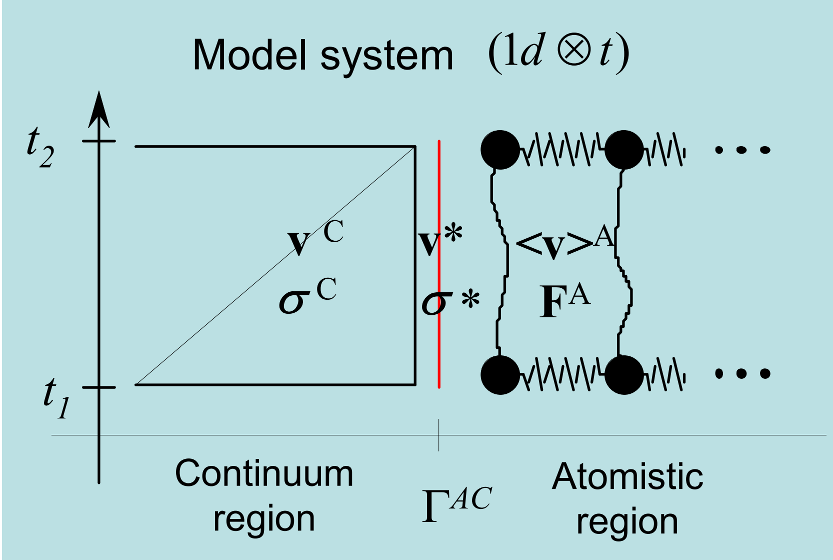


- Division of solution space into continuum and atomsitic regions remains constant $\Rightarrow$ $\mathbf{n}^{AC} \cdot \mathbf{e}_t = 0$
- No "ghost atoms" in continuum
- Currently implemented for 1*d* with 1st NN atom at boundary
- Implemented for aSDG with linear springs and VVerlet for linear springs and non-linear Morse potential (all 1NN)

Coupling: Atomistic and continuum SDG

- Continuum compatibility relations (kinematic and momentum)

$$\int_{\Gamma^{AC}} \left(\mathbf{v}^* - \mathbf{v}^C\right) \wedge \hat{\boldsymbol{\sigma}}^C$$
$$+ \int_{\Gamma^{AC}} \hat{\mathrm{v}}^C \cdot \left(\boldsymbol{\sigma}^* - \boldsymbol{\sigma}^C\right)$$



- Recall, $\mathbf{v}^*$ and σ^* are determined from values on both sides of interface.

- To supply flux conditions from atomistics,
  - homogenize atomic velocities at boundary $\langle\mathbf{v}\rangle^A$
  - solve for forces on atoms as initially undetermined forces

$$\int_{\Gamma^{AC}} \langle\hat{\mathbf{v}}\rangle^A \cdot \left(\boldsymbol{\sigma}^* - \mathbf{F}^A\right) + \int_{\Gamma^{AC}} \left(\mathbf{v}^* - \langle\mathbf{v}\rangle^A\right) \wedge \hat{\mathbf{F}}^A$$

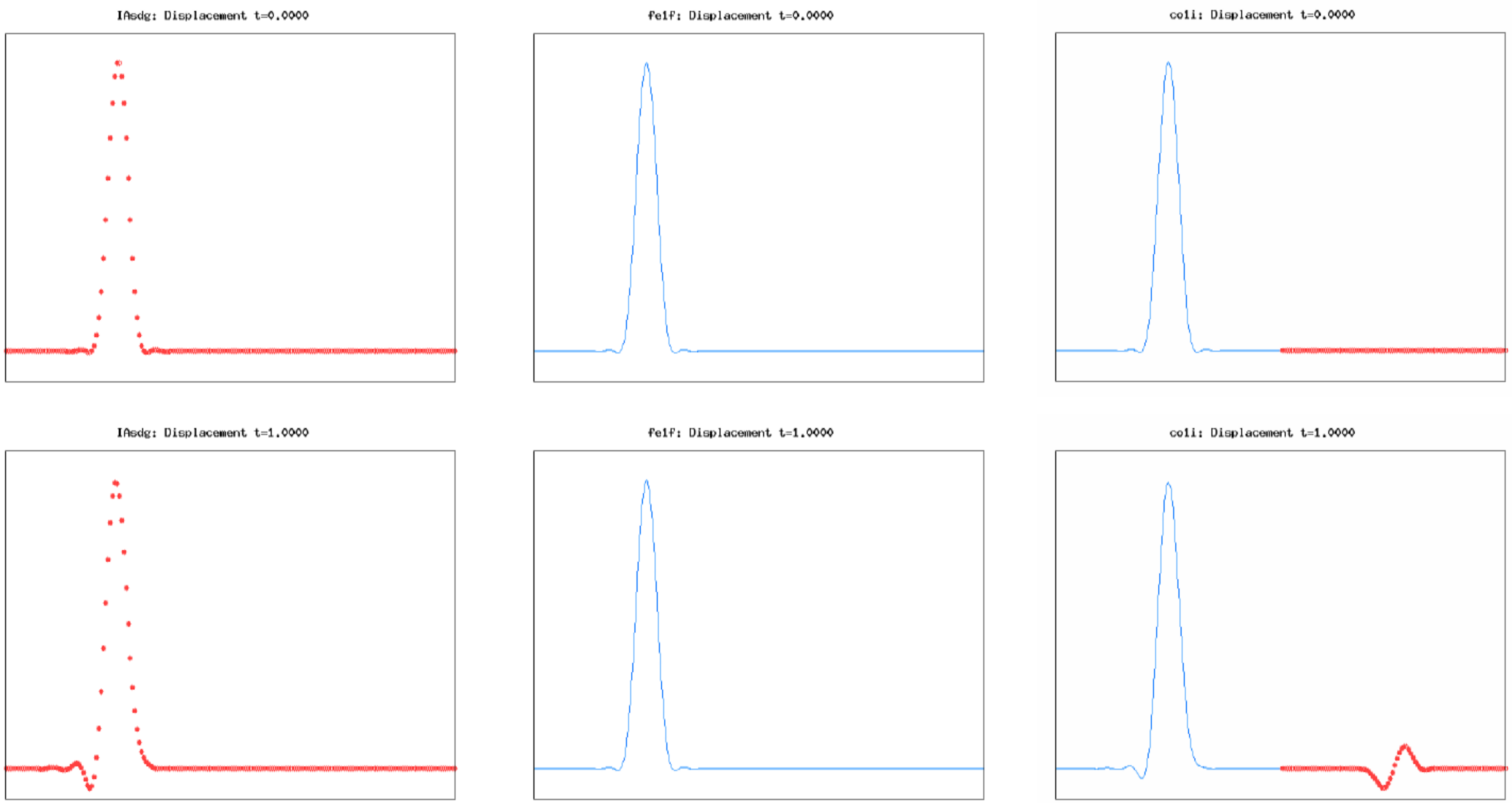
- Momentum balanced explicitly; Energy balance will depend on $\langle\mathbf{v}\rangle^A$

acSDG: Displacement error

Atomistic	Continuum	Coupled
200 atoms 5+4 dof	40 elements 5x5 dof	20 elements, 5x5 dof 100 atoms, 5+4 dof

Initial

After
1 pass



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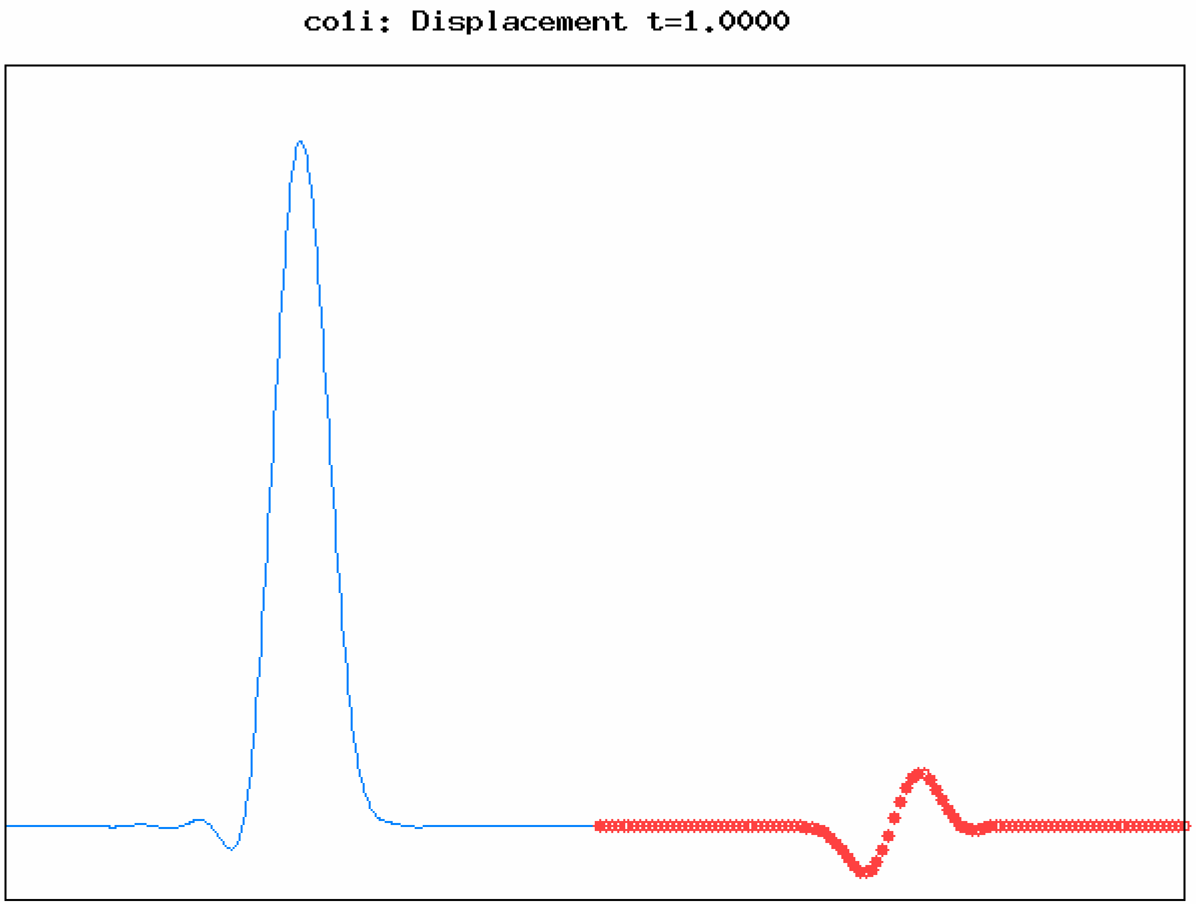
acSDG: Displacement error

Coupled: 20 elements, 5x5 dof ; 100 atoms, 5+4 dof

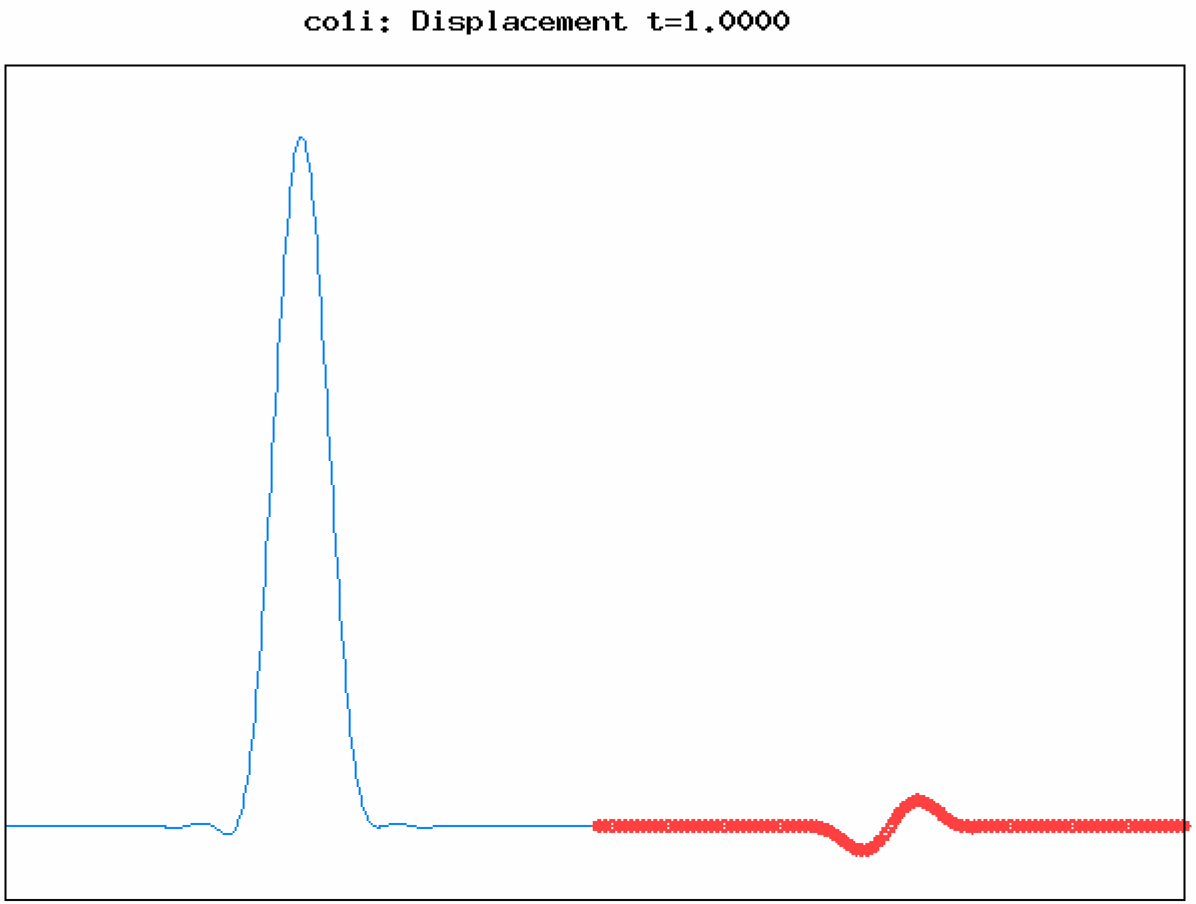
see external movie file: coupled100at.mov



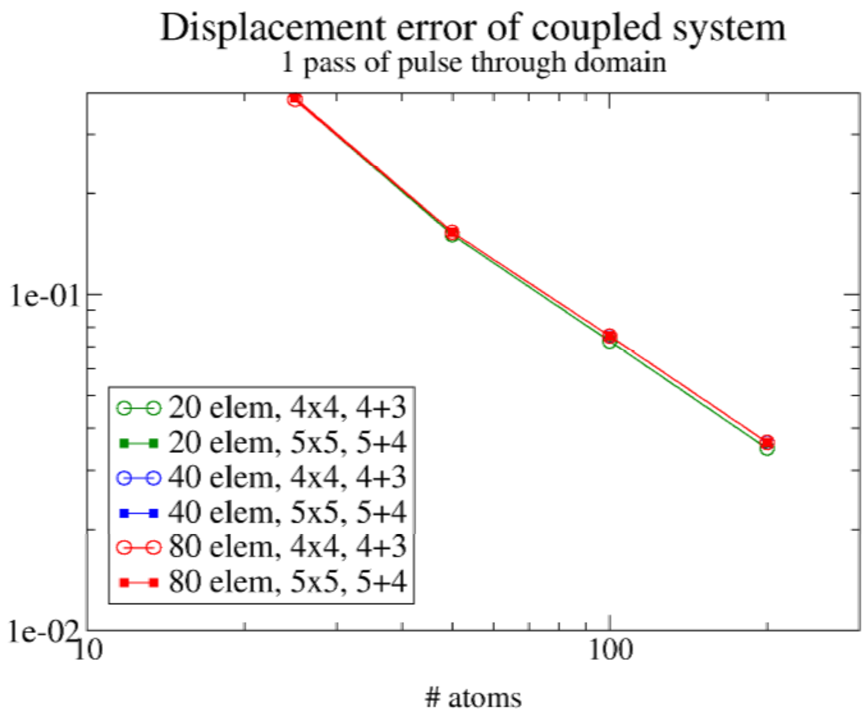
acSDG: Displacement error

Coupled: 20 elements, 5x5 dof ; 200 atoms, 5+4 dof

see external movie file: coupled200at.mov

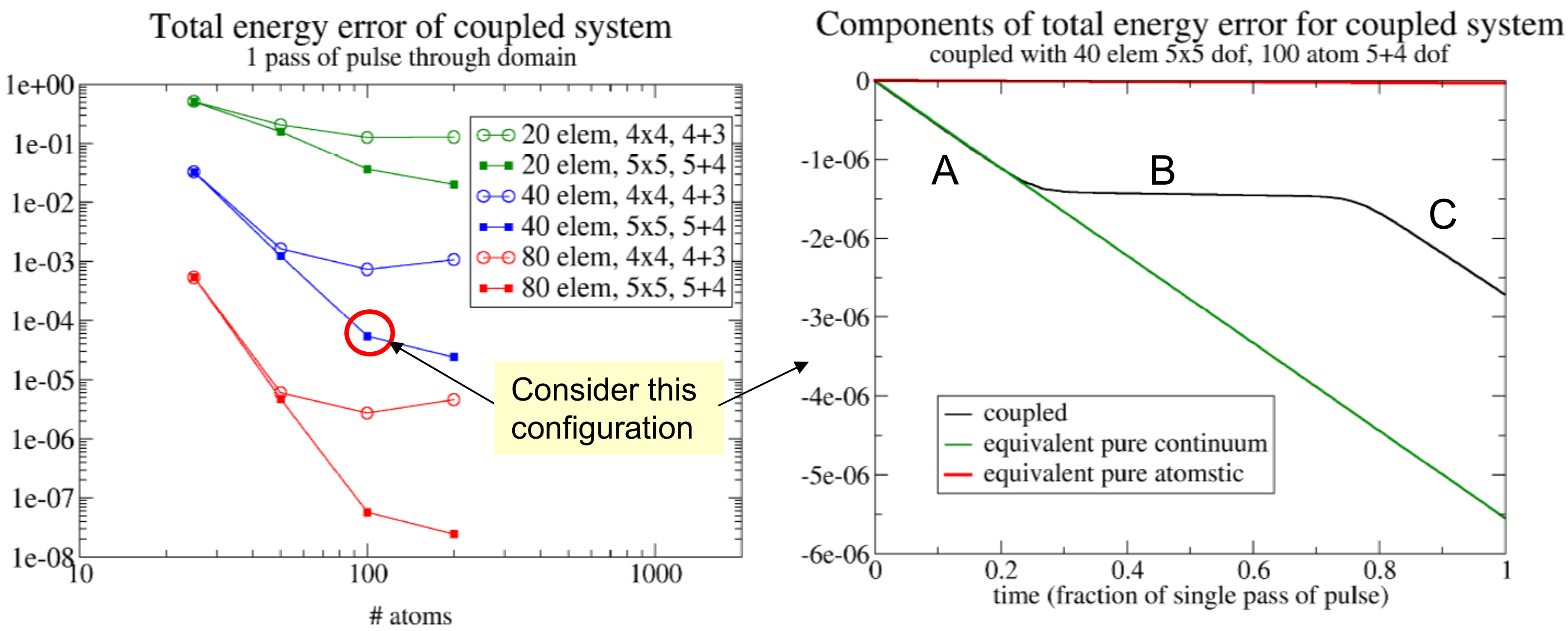


acSDG: Displacement error



- Displacement error scales with number of atoms
- Relative error due to number of elements and polynomial order insignificant in comparison

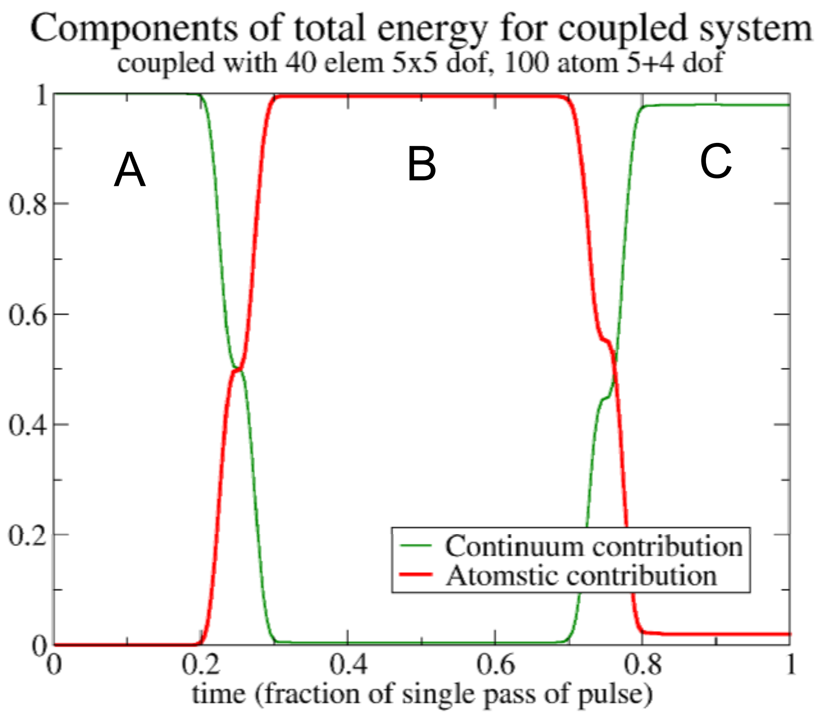
acSDG: Total energy error



A. Pulse begins in continuum region
B. Pulse fully in atomistic region
C. Pulse fully in continuum region

- Energy error reflects greater error component systems (atomistic or continuum)
- Similar trend seen in total momentum error

acSDG: Energy balance



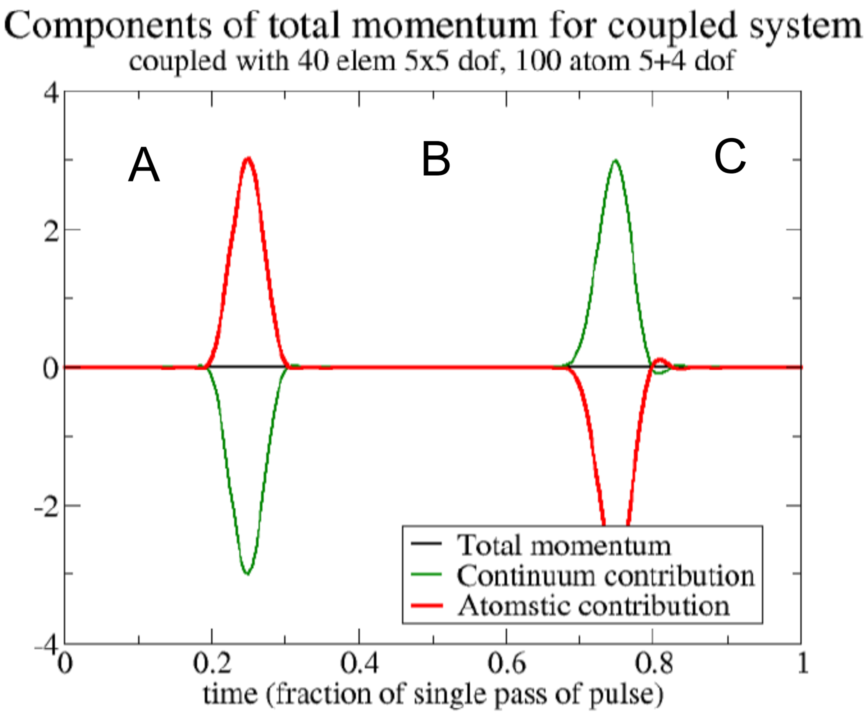
A. Pulse begins in continuum region
B. Pulse fully in atomistic region
C. Pulse fully in continuum region

- Slight energy error as pulse crosses interfaces

Component energy when pulse fully in one region

	t=0.0		t=0.5		t=1.0	
	Cont	At	Cont	At	Cont	At
20 elem, 100 at	1.0	0.0	5.0e-3	0.9948	0.9799	0.0196
40 elem, 100 at	1.0	0.0	5.0e-3	0.9950	0.9804	0.0196
20 elem, 200 at	1.0	0.0	1.2e-3	0.9984	0.9944	4.9e-3
40 elem, 200 at	1.0	0.0	1.2e-3	0.9988	0.9951	4.9e-3

acSDG: Momentum balance



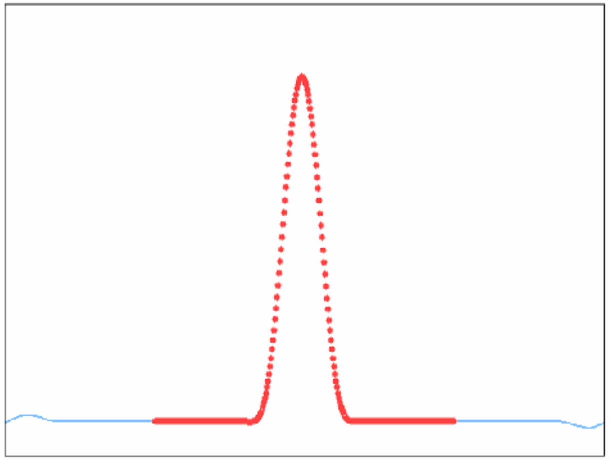
A. Pulse begins in continuum region
B. Pulse fully in atomistic region
C. Pulse fully in continuum region

- Total momentum ~10^{-10}
- Component momentum reflects pulse passing through coupling boundaries

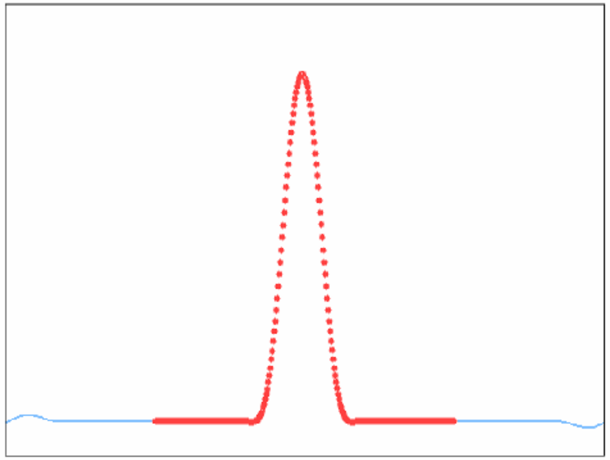
Component momentum when pulse fully in one region

	t=0.0		t=0.5		t=1.0	
	Cont	At	Cont	At	Cont	At
20 elem, 100 at	-4e-4	4e-4	5e-4	-5e-4	4e-4	-4e-4
40 elem, 100 at	-4e-4	4e-4	5e-4	-5e-4	4e-4	-4e-5
20 elem, 200 at	-2e-4	2e-4	3e-5	-3e-5	-3e-5	3e-5
40 elem, 200 at	-2e-4	2e-4	7e-5	-7e-5	-5e-5	5e-5

Coupling to V.Verlet with linear and non-linear potentials



1NN Linear spring



1NN Morse potential

- Results for VVerlet w/ 1NN spring effectively the same as aSDG
- Results for 1NN Morse potential effectively the same as 1NN spring for smallest

Coupled SDG summary

- Have shown a development of SDG FE method for both continuum discrete mechanics, focusing on differences
- Coupling achieved through flux conditions at AtC boundary
- Coupling employed aSDG in atomistic region (1NN linear spring)
- Similar results for VVerlet in atomistic region for linear spring and non-linear Morse potential (1NN)
- Currently 1*d* with 1NN interaction
- We have agreement between continuum and atomistics in continuum limit

Future research

- Higher order explicit approximations to aSDG
- Extending coupling in both dimension and interaction length
- Thermal coupling to appropriately handle reduction of d.o.f.